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Global sensitivity analysis in environmental water quality modelling: Where do we stand?

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Abstract: Global sensitivity analysis (GSA) is a valuable tool to support the use of mathematical models for environmental systems. During the last years the water quality modelling field has embraced the use of GSA. Environmental water quality modellers have tried to transfer the knowledge and experience acquired in other disciplines. The main objective of this paper is to provide an informed problem statement of the issues surrounding GSA applications in the environmental water quality modelling field. Specifically, this paper aims at identifying, for each GSA method, the potential use, the critical issues to be solved and the limits identified in a comprehensive literature review. The paper shows that the GSA methods are not mostly applied by using the numerical settings as suggested in the literature for other application fields. However, some authors have emphasized that the modeller must take care in employing such “default” numerical settings because, for complex water quality models, different GSA methods have been shown to provide different results depending on the settings. Quantitative convergence analysis has been identified as a key element for GSA quality control that merits further investigations for GSA application in the environmental water quality modelling field.

Keywords*:* Computational burden; convergence; modelling; numerical methods.

1. INTRODUCTION

Over the past 15 years the engineering and scientific communities in the environmental water quality modelling field have improved knowledge on the use of sensitivity analysis (SA). SA has been identified as a crucial step in any environmental modelling exercise (Jakeman et al., 2006). SAs have been conducted for several reasons: i. to identify factors that mainly influence specific model outputs of interest (*factor prioritization*); ii. to select which factors interact with each other (*interacting factors*); iii. to identify non-influential factors (*factor fixing*). Other possible objectives of GSA include *factors mapping* (to search which factors are responsible for producing outputs in a certain region, e.g. above a threshold value) or *variance cutting* (identify a minimal subset of factors to fix to obtain a prescribed reduction of uncertainty in the output) that are not explored in this analysis (Saltelli et al., 2004). Despite the nomenclature related to the objectives of GSA has explicitly been defined, literature shows the absence of a standardized nomenclature in using the different GSA methods.
By means of SA modellers are supported to identify critical regions in the factors’ space, to establish priorities for research and to simplify models (Saltelli et al., 2008).
Several SA methods have been proposed in literature, divided into two main groups: local sensitivity analysis (LSA) methods and global sensitivity analysis (GSA) methods (Saltelli, 2000). The LSA methods provide a measure of the local effect of input variation on the model outputs by varying the model factors with respect to a “nominal point” in the hyperspace of the input factors (Saltelli and Annoni, 2010). GSA methods assess how the model outputs are influenced by the variation of the model factors over their entire variation range (Homma and Saltelli, 1996; Saltelli et al., 2004).

In the environmental modelling field the majority of SA applications are local and derivative-based due to the fact that these methods are computationally very efficient (Saltelli et al., 2008). However, LSA methods can be misleading in case of non linear models due to the fact that they provide information only at the “nominal point”. Further, LSA does not allow identifying interacting or non-influential factors. Literature has shown that the main limits of LSA can be overcome by applying GSA. Indeed in case that the model behaviour is unknown a priori the GSA should be the preferred method to apply (Saltelli and Annoni, 2010). Saltelli et al. (2008) have classified GSA methods into: (i) global screening methods e.g. Morris screening method (Morris, 1991; Campolongo et al., 2007); (ii) variance-based methods such as Extended Fourier Amplitude Sensitivity Testing (Extended-FAST) (Saltelli et al., 2008), and (iii) regression/correlation-based methods such as the standardised regression coefficients (SRCs) method (Saltelli et al., 2008). However, due to the high complexity of environmental models, the spread of the GSA applications has been limited due to their high computational costs (Campolongo et al., 2007; Yang et al., 2011).

Despite such problems in applying GSA, recently modellers have spent considerable time in understanding the potential of each GSA method applied to complex models, especially in some areas such as hydrology (e.g., Massmann and Holzmann, 2012; Garambois et al., 2013; Herman et al., 2013; Zhan et al., 2013), urban drainage (Vezzaro and Mikkelesen, 2012; Donckels et al., 2013; Gamerith et al., 2013),wastewater treatment (Sin et al., 2011, Benedetti et al., 2011; Cosenza et al., 2013; Ramin et al., 2014) and drinking water treatment modelling (Neumann, 2012). In hydrology GSA methods have often been applied for evaluating the temporal patterns of factors sensitivity (Massmann and Holzmann, 2012; Garambois et al., 2013). All these GSA applications have emphasized several advantages of GSA and peculiarities of each method when applied to different models in terms of structure and number of factors involved.

In spite of the underlined advances of GSA, the applications found in literature have raised several critical issues, depending on the SA method applied and the peculiarities of the used mathematical model. However, it is important to underline that, as discussed below, the GSA applications found in literature show some disagreement especially in terms of required number of simulations (cost of analysis). Specifically different numerical settings are used applying the same method to different models.

For example: How can the terminology be standardized? Do all model applications require the same numerical settings for GSA? How should modellers test if the SA has converged? How to compare results when using multiple GSA methods? How can the computational cost be limited in the case of complex, over-parameterized non-linear and stiff models? These issues still need to be solved before reliable results can be guaranteed and these tools to enter mainstream use for the practitioner. The paper aims at providing the modeller the status about the application of GSA in the environmental water quality modelling field in order to summarize what he/she has to know before applying GSA.

2. TERMINOLOGY AND DEFINITIONS

Literature review on GSA shows that a generally accepted common GSA terminology permitting ease of comparison between the methods is still lacking (Mannina et al., 2012). Although Saltelli et al. (2004) provide a terminology in view of GSA *objectives* there is a missing terminology for comparing results in view of classification and cut-off levels for sensitivity indices obtained with different methods. Mannina et al. (2012) have recently provided the first attempt to standardize the GSA’s terminology for comparability of results by focusing the attention on three main methods: SRC, Morris screening and Extended-FAST.

We suggest classifying factors on the basis of a cut-off threshold (CT) for the sensitivity indices. Thus, after establishing the CT for β_i (CT_{SRC}), μ^*(CT_{MORRIS}), S_i ($CT_{E\text{-}FAST1}$), and S_{Ti} - S_i ($CT_{E\text{-}FAST2}$), the following classification has been provided for SRC, Morris screening and Extended-FAST methods:

- important factors: if sensitivity > CT_{SRC}
- important factors: if mean sensitivity > CT_{MORRIS}
- interacting factors: if mean sensitivity > CT_{MORRIS} and the standard deviation of the sensitivity is above a specified cone line
- non-influential factors: if mean sensitivity < CT_{MORRIS}
- important factors: if sensitivity > $CT_{E\text{-}FAST1}$
- interacting factors: if interaction > $CT_{E\text{-}FAST2}$
- non-influential factors: if sensitivity < $CT_{E\text{-}FAST1}$ and interaction < $CT_{E\text{-}FAST2}$

3. GSA METHODS

Table 1 summarizes the key features of the main GSA methods, that will be described in the sections below.
In particular, Table 1 summarizes for each method the ability to cope with interaction among factors and with non-linearity, the computational cost required to employ the analysis, the ability to provide information in terms of *factor fixing*, *factor prioritisation* and *variance cutting*. The symbols and the definitions in Table 1 are in accordance with Saltelli et al. (2008).

Table 1. Main features of GSA methods

		Features						Sensitivity measures	
Class	**Method**	**Coping with interaction**	**Coping with non linearity**	**Factor fixing**	**Factor prioritisation**	**Variance cutting**	**Cost of analysis**	**Symbol**	**Definition**
Regression/correlation	SRC	no	no	no	yes	no	500-1000	β_i	Standardised Regression Coefficient
Global screening	Morris screening	yes	yes	yes	no	no	r×(n+1)	μ	Mean of elementary effects
								μ^*	Mean of absolute elementary effects
								σ	Standard deviation of elementary effects
Variance based	Extended-FAST	yes	yes	yes	yes	yes	N× n	S_i	First order effect
								S_{Ti}	Total effect
	Sobol'	yes	yes	yes	yes	yes	N×(n+2)	S_i	First order effect
								S_{Ti}	Total effect
Where: n = number of factors; r = number of repetitions or trajectors, typically 4 ≤ r ≤ 10; N = number of repetitions, typically 500 ≤ N ≤ 1000									

3.1 Regression/correlation based methods

The rationale of regression/correlation based methods is to perform Monte Carlo (MC) simulations of the model output by using a randomly sampled factor matrix. Multivariate linear regression is then used relating model outputs to the factors (Saltelli et al., 2008). For each factor the standardised regression coefficient (SRC = β_i) of the multivariate linear model is calculated. β_i is a valid measure of sensitivity if the coefficient of determination R^2 is higher than 0.7 (Saltelli et al., 2008). In terms of computational demand regression/correlation methods are feasible to be used even for complex models with tens of factors. Indeed, the application of these methods requires a limited number of MC simulations, typical numbers found in literature are between 500 and 1000 (Neumann, 2012). However, the regression/correlation based methods explore only the 1st order effects and do not provide any information about the interaction among factors. Thus, these methods can be used only for *factor prioritization* in cases when the effects of non-linearity are not too strong ($R^2 > 0.7$).

3.2 Global screening methods

The Morris screening method represents the most used method belonging to the class of global screening methods. It is based on a one-at-a-time (OAT) perturbation of the model factors under investigation (Morris, 1991). For each perturbation the elementary effect (EE) is quantified. The EE represents the relative difference of the model output with and without a perturbation Δ of the ith factor. The EE is repeatedly computed (r times) at different locations in factors' space. For each of the n factors, the measure of sensitivity is summarized by the mean (μ) and the standard deviation (σ) of the cumulative distribution function of the EEs (generated by performing r replicates). μ represents a measure of the importance of the factor in determining model output whereas σ indicates whether the factor is responsible for introducing non-linearity or interactions (i.e. whether the sensitivity changes for different locations in factors space) (Table 1). In order to avoid the problem that EE's of opposite sign cancel each other out, Campolongo et al. (2007) proposed to use the mean of the absolute EEs (μ^*). The main objective of the Morris screening method is *factor fixing*: factors with low value of μ^* or σ are considered non important and can be fixed anywhere in the factor space. As suggested by Campolongo et al. (2007) the required number of simulations for the Morris screening application is equal to r*(n+1).

3.3 Variance-based methods

Variance-based methods are founded on the variance decomposition theorem that states that "the variance can be decomposed into conditional variances". Saltelli et al. (2008) summarized the main interesting features of variance based methods: i. independence of the model structure; ii. capability to analyse the influence of each factor within its entire range; iii. capability to quantify the interaction among factors, and iv. groups of factors can be considered as single factors. However, the main disadvantage of these methods is their computational cost as require a large number of simulations per factor (500-1000 according to Saltelli et al., 2005). In the application of variance based methods, modellers are often interested in two sensitivity indices: the first order effect index (S_i) and the total effect index (S_{Ti}) (Table 1). S_i measures how the ith factor contributes to the variance of the model output without taking into account the interactions among factors while S_{Ti} also considers the interactions among factors. Thus, the difference between S_{Ti} and S_i quantifies the interaction among factors (S_{Si}). Variance-based methods allow identifying important factors (high S_i) (*factors prioritization*). Only if S_{Ti} is small the factor be fixed anywhere within its range of uncertainty (*factor fixing*). Indeed, if the S_i value is small, it does not necessarily mean that the factor may be fixed because a high S_{Ti} value would indicate that the factor is involved in interactions. The most frequently used methods are: Extended-FAST and Sobol' (Cukier et al., 1973; Schaibly and Shuler, 1973; Sobol', 1993; Saltelli et al., 1999; Saltelli, 2002).

4. RESEARCH ON GSA

All the main relevant studies on GSA, found in literature, have been analysed. The studies are mainly referring to the fields of interest in this work: hydrology, water quality, wastewater and urban drainage.

In the field of wastewater modelling Sin et al. (2011) applied the SRC method in view of uncertainty analysis of a conventional activated sludge system model, in which three different scenarios were analyzed by taking into account 26, 7 and 33 factors respectively. The study of Sin et al. (2011) was aimed at selecting the most significant factors that contribute to the uncertainty of performance criteria (e.g. effluent quality, sludge production and energy consumption). For each scenario, different model inputs (such as biokinetic model parameters, influent fractions, mass-transfer parameters and the like), were considered to be uncertain or known. They found a high ability of the SRC method in identifying the main sources of uncertainty and quantifying their impact on process performance criteria. Chen et al. (2012) and Cosenza et al. (2013) found that complex models of membrane bio-reactors can be highly nonlinear by which the SRC method is jeopardized, and that variance based sensitivity analysis methods are required.
In the field of urban drainage Vezzaro and Mikkelsen (2012) applied a variance decomposition method combined with the general likelihood uncertainty estimation GLUE in order to identify the major sources of uncertainty in a stormwater quality model. Similarly to the other variance based applications Vezzaro and Mikkelsen (2012) have emphasized both the potential of these methods (e.g. coping with interaction and non linearity) and the drawback related to the high computational demand.

In order to select the appropriate method for the model under study several authors have tried to verify the potential of the different methods when applied to the same model. Indeed, some of the studies found in literature refer to the comparison of different GSA methods (Tang et al., 2007; Yang, 2011; Randrianantoandro et al., 2012; Sun et al., 2012; Neumann, 2012; Cosenza et al., 2013; Gamerith et al., 2013; Wainwright et al., 2014; Vazquez-Cruz et al., 2014). The comparison studies show that no standardized criteria for comparing the results obtained between different methods in terms of *factor fixing* and *factor prioritization* have yet been established. Hence the findings deduced from one study are often affected by the subjective choice of the modeller during the analysis making it difficult to apply for other models.
Most of the comparison studies show that similar results, mainly in terms of factor ranking, are obtained when different GSA methods are applied to a model with a low number of factors (Tang et al., 2007; Yang, 2011; Sun et al., 2012; Neumann, 2012; Gamerith et al., 2013; Wainwright et al., 2014). On the other hand especially in case of complex models, characterised by tens of model factors, relevant differences were found among the results.
Indeed, in the field of **wastewater modelling**, Cosenza et al. (2013) comparing SRC, Morris screening and Extended-FAST methods for a membrane bioreactor wastewater treatment model showed a poor similarity between Morris screening and Extended-FAST results in terms of both the

number and type of influential/non-influential factors. Cosenza et al. (2013) identified convergence problems for the Morris screening underlining the need to guarantee convergence when applying GSA methods, especially in case of complex models.

In water quality modelling Neumann (2012) compared five SA methods (derivative-based local sensitivity analysis, Morris Screening, SRC, Extended-FAST and an entropy-based method) applied to a drinking water model. Author found the same parameter ranking results for the different methods. However, for chemicals leading to high non-linearity, the approximation of 1st order effect indices using the local methods or regression-based methods was poor and classification differed among methods.

In hydrology Randrianantoandro et al. (2012) conducted an extensive comparison of different GSA methods (SRC, Morris and Extended-FAST) on a range of hydrological models applied to different reference catchments and found significant differences in the *factors fixing* results for some catchments whereas for others the results were equal. Randrianantoandro et al. 2012 showed contrasting results when the SRC, Morris screening and Extended- FAST methods (after testing convergence) were applied to the GR4J model (Perrin et al., 2003) and to the MORDOR 10 model (Paquet, 2004). As these latter models involved a low number of factors (4 and 10, respectively) authors concluded that the GSA methods don't always give the same grouping of factors.More recently, Gan et al. (2014) conducted a comprehensive analysis of the effectiveness of different sensitivity analysis methods for a very simple conceptual hydrologic model - Sacramento Soil Moisture Accounting (SAC-SMA) model (Burnash et al.,1973). Gan et al. (2014) found that the Morris screening method is not robust for various combinations of p and r values. Moreover, Massmann and Holzmann (2012) have applied three GSA methods (Sobol's indices, the mutual entropy and regional sensitivity analysis) for different temporal scales of evaluation ranging from daily to a multiannual period. They found that all methods are suitable for identifying the most important model factors. However, increasing differences in the results were obtained when the factors become less important and also when shorter temporal scales are considered (Massmann and Holzmann, 2012).

4.1 GSA applications dealing with convergence analysis

From the literature review one can observe that only a few studies present an analysis of convergence of the GSA (Tang et al., 2007; Benedetti et al., 2011; Yang, 2011; Dotto et al., 2012; Wang et al., 2013; Wainwright et al., 2014; Vazquez-Cruz et al., 2014).

In the field of hydrology Yang (2011) proposed a method to investigate the convergence of the results of different Monte Carlo based GSA methods by using two techniques: the Central Limit Theorem and the bootstrap technique. Yang (2011) found that for each GSA method applied the bootstrap technique leads to a lower number of simulations required than the Central Limit Theorem.

In the field of wastewater modelling Benedetti et al. (2011) proposed a method to reduce the computational cost of Monte Carlo based GSA methods. The authors used two criteria (the model output variability and the stability of the composition of the important factor set as the number of iterations increases) to select the minimum number of simulations to be performed. They found that depending on the analysed variable the results of the convergence analysis vary, highlighting that the achievement of convergence is strongly dependent on the model output considered during GSA application. Ruano et al. (2012) investigated the convergence of Morris screening results for a wastewater treatment plant model. They proposed a criterion (the position factor) for establishing the achievement of convergence. By increasing the number of replicates (r) of the OAT sampling from 5 to 70, Ruano et al. (2012) analysed the average variation of the sum of the rank of the model factors (position factor). Ruano et al. (2012) found that the optimal number of repetitions was 60-70, which is considerably higher than recommended by Saltelli et al. (2008) (namely 4-10 as reported in Table 1). The work of Ruano et al. (2012) confirmed that the modeller must take care in employing such "default" numerical settings proposed in literature especially in case of complex models.

In other fields Wang et al. (2013) investigated the convergence of sensitivity measures for a **crop growth model** by applying the Extended-FAST method. The authors suggest using a small factor sample size in case the modeller is interested only in factor rankings. On the other hand Wang et al. (2013) corroborated the fact that the factor variation range strongly influences the sensitivity value of the most important factors. Recently, Loeppky et al. (2013) discussed the relationship between sensitivity analysis and the dimension of the factors space for the probabilistic sensitivity analysis method based on the Gaussian process model by using Latin Hypercube Sampling. Loeppky et al. (2013) found that in case of **protein and ocean circulation models** the number of simulations

required for having a desired level of accuracy of model predictions is ten times the number of factors evaluated.
The literature review on convergence analysis shows that despite the fact that researchers having attempted in several ways to evaluate the convergence of GSA methods, it remains an open issue. As far as we know, no pragmatic rule has yet been defined to guarantee convergence of GSA outputs.

4.2 Complementary use of multiple GSA methods

The choice of the GSA method to apply is not always clear a priori due to unknown model behaviour. By applying different GSA methods modellers can obtain different types of information about the effects of each factor on the model output. Several authors have underlined that only by applying different methods simultaneously, a thorough analysis of the impact of model factors on the model outputs and the model's degree of nonlinearity can be obtained (Schouten et al., 2014, Neumann 2012). Further, in case of non-linear models, literature suggests the use of global screening or variance-based methods (Table 1). However, these methods require a large number of simulations thus increasing the computational time required for the analysis. The computational time becomes an even more limiting factor in case of dynamic, complex, large and stiff systems. Thus, according to Saltelli et al. (2008), in case of complex models, a complementary use of different GSA methods is suggested in order to reduce the number of factors to consider before applying high computational demanding methods as Extended-FAST. However, to ensure that this procedure works, one must ascertain that no factors are eliminated wrongly.
With this regard Sun et al. (2012) suggested to use, in case of a model with a large number of factors, a two-step procedure including first a factors screening step (by using a local method) followed by a GSA step of the important factors identified during the first step. Moreau et al. (2013) have applied a two step GSA for a spatially-distributed agro-hydrological model (first Morris screening method and then ANOVA). Further, Vanuytrecht et al. (2014) used first Morris screening and then Extended-FAST method. Recently, Gan et al. (2014) have suggested in case of complex models to use first approximate methods (e.g. SRC or local methods) for a rough factor screening and then quantitative methods as Extended-FAST or Sobol's methods.
However, despite the advantage of the complementary use of different GSA methods several questions need to be addressed: Is this really an effective practice for overcoming computational burden?

5. CONCLUSIONS AND ISSUES THAT NEED FURTHER INVESTIGATIONS

This paper has outlined the issues surrounding the GSA in the environmental water quality modelling field. In particular, the literature review on GSA methods has provided several issues that need further investigation in order to improve the application in water quality modelling field:

- standardized criteria and terminology to compare results of different GSA method should be established; the authors have made a first proposal.
- Considerable variability was found in the numerical settings applied (number of simulations) between different GSA studies. Pragmatic rules or procedures are required to support the modeller in determining how many simulations need to be run to achieve convergence of the outcomes of the GSA analysis.
- The results of the GSA analysis in terms of factors fixing and factors prioritisation are also found to depend on the GSA method applied, thus asking for a better understanding of how the methods need to be applied and how to interpret the results.

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